Appendix B:
Environmental Fate Data

Environmental Fate

No environmental fate data which could be considered fully acceptable under Subdivision N Guidelines have been submitted to the Agency for Avitrol. However, after perusing the readily available open literature and structural analysis sources of information, EFED expects Avitrol to be both mobile and persistent in the open environment. The main route of dissipation for Avitrol (4-aminopyridine) in the environment is assumed to be through aerobic metabolism. No data concerning any possible transformation/degradation properties of Avitrol have been submitted to the Agency.

Persistence

The prediction of persistence for Avitrol is based upon ancillary, pre-Subdivision N data submissions for Avitrol (~1970-1975). Abiotic half-life values could not be derived from submitted data, and the assumption of stability has been made for both hydrolysis and photolysis of Avitrol. Although an anaerobic metabolism half-life value could not be calculated, submitted data were sufficient to determine that Avitrol can be considered stable under anaerobic conditions[1]. The submitted studies can not be considered fully acceptably because they contain no data concerning either the identity or the environmental fate properties of any potential degradation products of 4-aminopyridine. Additionally, study results were presented in terms of evolved radio labeled CO_2, and not in terms of half-lives calculated from log transformed data. Under aerobic conditions, half-life values ranged between 3 and 32 months[2]. Information about soil types, storage stability, degradation products, and even individual half-lives is absent from this supplemental study. These biotic half-lives are consistent with structural analysis model predictions from EPI Suite (v3.12) fugacity calculations. The EPI Suite level III fugacity model half-life predicts an aerobic metabolism half-life of 75 days (2 ½ months), and an anaerobic metabolism half-life of about one year for 4-aminopyridine.

EPI Suite (v3.12) fugacity calculations predict that the combined percents of Avitrol partitioning into the air and sediments in the open environments would be slightly greater than 0.1%. This is consistent with available data. While both the vapor pressure and the Henry's Law Constant are relatively high for a pesticide, the aqueous solubility is unusually high at the grams per liter range. This high aqueous solubility along with the low octanol/.water partitioning coefficient suggests that Avitrol will have a low potential to bioaccumulate in the fatty tissues of fish. The EPI Suite model goes on to predict that less than 2% of 4-aminipyridine concentrations will be removed by wastewater treatment.

Aquatic metabolism data are not available for use in this assessment.

Transport

The prediction of mobility for Avitrol can not be based upon ancillary, pre-Subdivision N data submissions for Avitrol. Revisiting the old data submissions (MRID No. 05003185) reveled that the mobility study is unacceptable under current standards.

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[1] MRID No. 05003185

[2] EPI Suite (v3.12) PCKOCWIN (v1.6)

Columns packed with soil were leached with water, which is known to collapse soil structure. This phenomenon is known to be capable of making even mobile pesticides appear to bind strongly to soil.

The prediction of mobility for Avitrol is based upon high aqueous solubility (112 g/L)[3], a low octanol/water partitioning coefficient value (log K_{ow} = -0.74)[4], and a low structural analysis modeled soil/water partitioning coefficient value (K_{oc} = 44.8)[5]. This prediction of mobility, along with the prediction of persistence, suggests that Avitrol does possess the potential to reach ground water.

On the other hand, given a general understanding of soil structuring[6] and pyridine chemistry[7], EFED can not rule out the possibility that Avitrol might also be susceptible to aged sorption.

While the vapor pressure (2.09 x 10^{-4} mm Hg)[8] and Henry's Law Constant (2.4 x 10^{-9} atm - m^3/mole)[9] of 4-aminopyridine indicate that there is some potential for the pure compound to volatilize, EFED believes that bait which has been pretreated with Avitrol would not volatize appreciably. Pure pyridine derivatives have a distinctively pungent odor which would not generally be considered appetizing. If 4-aminopyridine did volatize from the treated bait, it is reasonable to expect it to render the treated bait less palatable, making the product less effective.

No monitoring data could be located for Avitrol (4-aminopyridine) using: the USGS online NAWQA (National Water Quality Assessment Data Warehouse) database,[10] EPA monitoring publication,[11] and the Google internet search engine.[12]

Transformation

Except for radio labeled carbon dioxide evolved from the biotic metabolism studies,[13] no data concerning the quantity, the identity or the environmental fate properties of any potential degradation products of 4-aminopyridine are available to EFED. 4-Aminopyridine[14] (Avitrol), like other heteroaromatic nitrogen compounds, is expected to be susceptible to nucleophillic substitution in the ortho and para positions[15]. 4-Aminopyridine consists of a pyridine ring, with an amino group in the para position. With two nitrogen atoms present in this heterocyclic molecule, the stabilization to the

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[3] MRID No. 40603603
[4] MRID No. 40603603
[5] EPI Suite (v3.12) PCKOCWIN (v1.6)
[6] *The Chemistry of Soils*, pps. 25-33
[7] *Advanced Organic Chemistry, 3rd edition, part A: Structure and Mechanisms*, p. 583.
[8] MRID No. 40603603
[9] EPI Suite (v3.12) HENRYWIN (v3.10)
[10] http://infotrek.er.usgs.gov/traverse/f?p=NAWQA:HOME:16059544255308576875
[11] EPA Pesticides in Ground Water, A Compilation Of Monitoring Studies: 1971 – 1991 National Summary
[12] keywords: Avitrol or 4-aminopyridien, and monitoring or water or study
[13] MRID No. 05003185
[14] *Advanced Organic Chemistry, Reaction, Mechanisms, and Structures*, 4th edition, pps. 3552-355.
[15] *Organic Chemistry*, 4th edition, pps. 933-936.

addition intermediate is expected to be enhanced, further activating the aromatic ring to nucleophillic attack. Considering the complex and varied structuring of soils[16], it would be difficult to predict degradation products from nucleophillic substitution. Therefore, degradates were not addressed in this assessment.

Bioaccumulation

Bioconcentration in fish data are not available for either Avitrol, or any potential degradation products. The low log K_{ow} value gleaned from the open literature suggests that Avitrol would not be expected to bioaccumulate in fish.

Table B-1 Summary of Environmental Fate Properties of Avitrol Used in Assessment

Study Type	Value	Source / MRID Number
Hydrolysis	half-life = assumed stable	unable to estimate through EPI Suite, no acceptable data are available
Aquatic Photodegradation	half-life = assumed stable	unable to estimate through EPI Suite, no acceptable data are available
Photodegradation on Soil	half-life = assumed stable	unable to estimate through EPI Suite, no acceptable data are available
Aerobic Soil Metabolism	half-lives = 3 to 32 months[1]	MRID No. 05003185 (supplemental study)
Aerobic Aquatic Metabolism	half-life = assumed stable	unable to estimate through EPI Suite, no acceptable data are available
Anaerobic Aquatic Metabolism	half-life = stable[1]	MRID No. 05003185 (supplemental study)
Adsorption/Desorption	K_{oc} = 44.8	EPI Suite (v3.12; value consistent with literature aqueous solubility[2] and K_{ow}[3] data)
Bioaccumulation in Fish	assumed not to bioconcentrate	based upon literature log K_{ow}[3] data (0.26)
Terrestrial Field Dissipation	half-life = unknown	unable to estimate through EPI Suite, no acceptable data are available

1 = soils used in test systems unknown
2 = EPI Suite (v3.12) experimental database match (reference: BEILSTEIN)
3 = EPI Suite (v3.12) experimental database match (reference: Hansch, C et al. 1955)

[16] *Environmental Soil Chemistry*, pps. 31-43.

EPI Suite (v3.12) Output

```
SMILES : n(ccc(N)c1)c1
CHEM   : 4-Pyridinamine
CAS NUM: 000504-24-5
MOL FOR: C5 H6 N2
MOL WT : 94.12
------------------------------ EPI SUMMARY (v3.12) --------------------
------
 Physical Property Inputs:
    Water Solubility (mg/L):   ------
    Vapor Pressure (mm Hg) :   ------
    Henry LC (atm-m3/mole) :   ------
    Log Kow (octanol-water):   ------
    Boiling Point (deg C)  :   ------
    Melting Point (deg C)  :   ------

KOWWIN Program (v1.67) Results:
================================

                  Log Kow(version 1.67 estimate): -0.11

Experimental Database Structure Match:
  Name     :  4-Aminopyridine
  CAS Num  :  000504-24-5
  Exp Log P:  0.26
  Exp Ref  :  Hansch,C et al. (1995)

SMILES : n(ccc(N)c1)c1
CHEM   : 4-Pyridinamine
MOL FOR: C5 H6 N2
MOL WT : 94.12
-------+-----+-----------------------------------------+---------+--
------
 TYPE  | NUM |        LOGKOW FRAGMENT DESCRIPTION         |  COEFF  |
VALUE
-------+-----+-----------------------------------------+---------+--
------
 Frag  |  5  |  Aromatic Carbon                          | 0.2940  |
1.4700
 Frag  |  1  |  Aromatic Nitrogen                        |-0.7324  | -
0.7324
 Frag  |  1  |  -N    [aliphatic N, one aromatic attach] |-0.9170  | -
0.9170
 Factor|  1  |  Pyridine ring (non-fused)  correction    |-0.1621  | -
0.1621
 Const |     |  Equation Constant                        |         |
0.2290
-------+-----+-----------------------------------------+---------+--
------
                                                        Log Kow   =  -
0.1125



MPBPWIN (v1.41) Program Results:
```

```
================================
Experimental Database Structure Match:
  Name     :  4-AMINOPYRIDINE
  CAS Num  :  000504-24-5
  Exp MP (deg C):  158.5
  Exp BP (deg C):  273
  Exp VP (mm Hg):  ---

SMILES : n(ccc(N)c1)c1
CHEM   : 4-Pyridinamine
MOL FOR: C5 H6 N2
MOL WT : 94.12
----------------------- SUMMARY MPBPWIN v1.41 --------------------


Boiling Point:  193.56 deg C (Adapted Stein and Brown Method)

Melting Point:   54.17 deg C (Adapted Joback Method)
Melting Point:   -0.64 deg C (Gold and Ogle Method)
Mean Melt Pt :   26.76 deg C (Joback; Gold,Ogle Methods)
  Selected MP:   26.76 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
  (Using BP: 273.00 deg C (exp database))
  (Using MP: 158.50 deg C (exp database))
    VP:  0.000325 mm Hg (Antoine Method)
    VP:  0.000347 mm Hg (Modified Grain Method)
    VP:  0.000703 mm Hg (Mackay Method)
  Selected VP:  0.000347 mm Hg (Modified Grain Method)


-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  4  |  CH (aromatic)     |   28.53  |  114.12
 Group |  1  |  -C (aromatic)     |   30.76  |   30.76
 Group |  1  |  -NH2 (to arom)    |   86.63  |   86.63
 Group |  1  |  N (aromatic)      |   39.88  |   39.88
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  469.57
RESULT- corr |  BOILING POINT in deg Kelvin  |  466.72
             |  BOILING POINT in deg C       |  193.56
-----------------------------------------------------


-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  4  |  CH (aromatic)     |    8.13  |   32.52
 Group |  1  |  -C (aromatic)     |   37.02  |   37.02
 Group |  1  |  -NH2 (to arom)    |   66.89  |   66.89
 Group |  1  |  N (aromatic)      |   68.40  |   68.40
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  327.33
             |  MELTING POINT in deg C       |   54.17
-----------------------------------------------------
```

```
Water Sol from Kow (WSKOW v1.41) Results:
==========================================

          Water Sol: 7.285e+004 mg/L

Experimental Water Solubility Database Match:
  Name     :  4-AMINOPYRIDINE
  CAS Num  :  000504-24-5
  Exp WSol :  8.33E+004 mg/L (20 deg C)
  Exp Ref  :  BEILSTEIN

SMILES : n(ccc(N)c1)c1
CHEM   : 4-Pyridinamine
MOL FOR: C5 H6 N2
MOL WT : 94.12
---------------------------------- WSKOW v1.41 Results ----------------
--------
Log Kow  (estimated)  :  -0.11
Log Kow (experimental):  0.26
    Cas No: 000504-24-5
    Name  : 4-Aminopyridine
    Refer : Hansch,C et al. (1995)
Log Kow used by Water solubility estimates:  0.26

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      --------------------   -----
       No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :  -0.111
   Water Solubility at 25 deg C (mg/L):  7.285e+004



WATERNT Program (v1.01) Results:
================================

                  Water Sol (v1.01 est): 1e+006 mg/L

Experimental Water Solubility Database Match:
  Name     :  4-AMINOPYRIDINE
  CAS Num  :  000504-24-5
  Exp WSol :  8.33E+004 mg/L (20 deg C)
  Exp Ref  :  BEILSTEIN

SMILES : n(ccc(N)c1)c1
CHEM   : 4-Pyridinamine
MOL FOR: C5 H6 N2
MOL WT : 94.12
-------+-----+-------------------------------------------+----------+-
--------
```

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	4	Aromatic Carbon (C-H type)	-0.3359	-1.3435
Frag	1	Aromatic Nitrogen [max count of 1 allowed]	1.9255	1.9255
Frag	1	-N [aliphatic N, one aromatic attach]	1.2749	1.2749
Frag	1	Aromatic Carbon (C-substituent type)	-0.5400	-0.5400
Const		Equation Constant		0.2492
NOTE		Maximum Solubility (1,000,000 mg/L) Applied!		

Log Water Sol (moles/L) at 25 dec C = 1.0263

Water Solubility (mg/L) at 25 dec C = 1e+006

ECOSAR Program (v0.99h) Results:
==========
SMILES : n(ccc(N)c1)c1
CHEM : 4-Pyridinamine
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C5 H6 N2
MOL WT : 94.12
Log Kow: -0.11 (KowWin estimate)
Melt Pt:
Wat Sol: 5.941E+004 mg/L (calculated)

ECOSAR v0.99h Class(es) Found

Aromatic Amines

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR	Fish	14-day	LC50	8699.166
(Baseline Toxicity)				
Aromatic Amines	Fish	96-hr	LC50	1025.552

```
Aromatic Amines            : Fish                14-day    LC50
1265.749
Aromatic Amines            : Daphnid             48-hr     LC50
2.401
Aromatic Amines            : Fish                          ChV
3.361
Aromatic Amines            : Daphnid                       ChV
0.078
Aromatic Amines            : Green Algae                   ChV
42.398

 Note:  * = asterisk designates: Chemical may not be soluble
        enough to measure this predicted effect.
         Fish and daphnid acute toxicity log Kow cutoff: 7.0
         Green algal EC50 toxicity log Kow cutoff: 7.0
         Chronic toxicity log Kow cutoff: 9.0
         MW cutoff: 1000



HENRY (v3.10) Program Results:
==============================

       Bond Est :  2.49E-009 atm-m3/mole
       Group Est:  2.45E-009 atm-m3/mole

SMILES : n(ccc(N)c1)c1
CHEM   : 4-Pyridinamine
MOL FOR: C5 H6 N2
MOL WT : 94.12
--------------------------- HENRYWIN v3.10 Results --------------------
------
----------+---------------------------------------------+---------+----
------
   CLASS  |     BOND CONTRIBUTION DESCRIPTION           | COMMENT |
VALUE
----------+---------------------------------------------+---------+----
------
 HYDROGEN |   4  Hydrogen to Carbon (aromatic) Bonds    |         | -
0.6172
 HYDROGEN |   2  Hydrogen to Nitrogen Bonds             |         |
2.5670
 FRAGMENT |   4  Car-Car                                |         |
1.0552
 FRAGMENT |   2  Car-Nar                                |         |
3.2564
 FRAGMENT |   1  Car-N                                  |         |
0.7304
----------+---------------------------------------------+---------+----
------
 RESULT   |    BOND ESTIMATION METHOD for LWAPC VALUE   |  TOTAL  |
6.992
----------+---------------------------------------------+---------+----
------
HENRYs LAW CONSTANT at 25 deg C = 2.49E-009 atm-m3/mole
                                = 1.02E-007 unitless
```

```
--------+---------------------------------------------+------------+-
-------
        |        GROUP CONTRIBUTION DESCRIPTION       |   COMMENT  |
VALUE
--------+---------------------------------------------+------------+-
-------
        |           1  NH2 (Car)                      |  ESTIMATE  |
4.00
        |           1  Car (N)(Car)(Car)              |  ESTIMATE  |
-0.50
        |           2  Car-H (Car)(Car)               |            |
0.22
        |           2  Car-H (Car)(Nar)               |            |
0.22
        |           1  Nar (Car)(Car)                 |            |
3.06
--------+---------------------------------------------+------------+-
-------
 RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  |    TOTAL   |
7.00
--------+---------------------------------------------+------------+-
-------
HENRYs LAW CONSTANT at 25 deg C = 2.45E-009 atm-m3/mole
                                = 1.00E-007 unitless


Henrys LC [VP/WSol estimate using EPI values]:
    HLC:  5.899E-010 atm-m3/mole
    VP:   0.000347 mm Hg
    WS:   7.29E+004 mg/L



BIOWIN (v4.02) Program Results:
==============================
SMILES : n(ccc(N)c1)c1
CHEM   : 4-Pyridinamine
MOL FOR: C5 H6 N2
MOL WT : 94.12
--------------------------- BIOWIN v4.02 Results ----------------------
------

   Biowin1 (Linear Model Prediction)    :  Does Not Biodegrade Fast
   Biowin2 (Non-Linear Model Prediction):  Does Not Biodegrade Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Weeks-Months
   Biowin4 (Primary  Biodegradation Timeframe):  Days-Weeks
   Biowin5 (MITI Linear Model Prediction)    :  Does Not Biodegrade
Fast
   Biowin6 (MITI Non-Linear Model Prediction):  Does Not Biodegrade
Fast
   Ready Biodegradability Prediction:  NO

------+-----+-----------------------------------------+---------+---
------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION      |  COEFF  |
VALUE
```

Frag	1	Aromatic amine [-NH2 or -NH-]	-0.2338	-0.2338
Frag	1	Pyridine ring	-0.1546	-0.1546
MolWt	*	Molecular Weight Parameter		-0.0448
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		0.3144

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic amine [-NH2 or -NH-]	-1.9070	-1.9070
Frag	1	Pyridine ring	-1.6381	-1.6381
MolWt	*	Molecular Weight Parameter		-1.3365
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.1332

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic amine [-NH2 or -NH-]	-0.1349	-0.1349
Frag	1	Pyridine ring	-0.2142	-0.2142
MolWt	*	Molecular Weight Parameter		-0.2080
Const	*	Equation Constant		3.1992

```
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)  |         |
2.6421
============+============================================+=========+===
======

------+-----+--------------------------------------------+---------+---
------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION         |  COEFF  |
VALUE
------+-----+--------------------------------------------+---------+---
------
 Frag |  1  |  Aromatic amine   [-NH2  or  -NH-]         | -0.1084 | -
0.1084
 Frag |  1  |  Pyridine ring                             | -0.0187 | -
0.0187
 MolWt|  *  |  Molecular Weight Parameter                |         | -
0.1358
 Const|  *  |  Equation Constant                         |         |
3.8477
============+============================================+=========+===
======
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg)  |         |
3.5848
============+============================================+=========+===
======

 Result Classification:   5.00 -> hours     4.00 -> days    3.00 ->
weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer

------+-----+--------------------------------------------+---------+---
------
 TYPE | NUM |       Biowin5 FRAGMENT DESCRIPTION         |  COEFF  |
VALUE
------+-----+--------------------------------------------+---------+---
------
 Frag |  1  |  Aromatic amine   [-NH2  or  -NH-]         | -0.1577 | -
0.1577
 Frag |  1  |  Pyridine ring                             | -0.0335 | -
0.0335
 Frag |  4  |  Aromatic-H                                |  0.0082 |
0.0329
 MolWt|  *  |  Molecular Weight Parameter                |         | -
0.2800
 Const|  *  |  Equation Constant                         |         |
0.7121
============+============================================+=========+===
======
   RESULT   |  Biowin5 (MITI Linear Biodeg Probability)  |         |
0.2738
============+============================================+=========+===
======

------+-----+--------------------------------------------+---------+---
------
 TYPE | NUM |       Biowin6 FRAGMENT DESCRIPTION         |  COEFF  |
VALUE
```

```
------+-----+-----------------------------------------+---------+---
------
 Frag |  1  |  Aromatic amine   [-NH2  or  -NH-]      | -1.2264 | -
1.2264
 Frag |  1  |  Pyridine ring                          | -0.4599 | -
0.4599
 Frag |  4  |  Aromatic-H                             |  0.1201 |
0.4806
 MolWt|  *  |  Molecular Weight Parameter             |         | -
2.7170
============+=========================================+=========+===
======
   RESULT   |Biowin6 (MITI Non-Linear Biodeg Probability)|         |
0.1983
============+=========================================+=========+===
======

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades
Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast




AOP Program (v1.91) Results:
============================
SMILES : n(ccc(N)c1)c1
CHEM   : 4-Pyridinamine
MOL FOR: C5 H6 N2
MOL WT : 94.12
------------------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ------------
-------
Hydrogen Abstraction       =   0.0000 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =  20.4268 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  20.4268 E-12 cm3/molecule-sec
   HALF-LIFE =     0.524 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =     6.284 Hrs
------------------- SUMMARY (AOP v1.91): OZONE REACTION ---------------
-------

               ******  NO OZONE REACTION ESTIMATION ******
               (ONLY Olefins and Acetylenes are Estimated)

Experimental Database:  NO Structure Matches



PCKOC Program (v1.66) Results:
==============================

                   Koc (estimated): 44.8
```

Koc may be sensitive to pH!
SMILES : n(ccc(N)c1)c1
CHEM : 4-Pyridinamine
MOL FOR: C5 H6 N2
MOL WT : 94.12
---------- PCKOCWIN v1.66 Results ----------

First Order Molecular Connectivity Index ..... : 3.394
Non-Corrected Log Koc ..... :
2.4281
Fragment Correction(s):
* Nitrogen to non-fused aromatic ring ... : -
0.7770
Corrected Log Koc ..... :
1.6511

Estimated Koc: 44.78

NOTE:
The Koc of this structure may be sensitive to pH! The estimated Koc represents a best-fit to the majority of experimental values; however, the Koc may vary significantly with pH.

HYDROWIN Program (v1.67) Results:
==========
SMILES : n(ccc(N)c1)c1
CHEM : 4-Pyridinamine
MOL FOR: C5 H6 N2
MOL WT : 94.12
---------- HYDROWIN v1.67 Results ----------

Currently, this program can NOT estimate a hydrolysis rate constant
for
the type of chemical structure entered!!

ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3
halogens)
and Specific Alkyl Halides can be estimated!! For more information,
(Click OVERVIEW in Help or see the User's Guide)

***** CALCULATION NOT PERFORMED *****

BCF Program (v2.15) Results:
==========
SMILES : n(ccc(N)c1)c1
CHEM : 4-Pyridinamine
MOL FOR: C5 H6 N2
MOL WT : 94.12

---------- Bcfwin v2.15 ----------

Log Kow (estimated) : -0.11
Log Kow (experimental): 0.26
Log Kow used by BCF estimates: 0.26

Equation Used to Make BCF estimate:
   Log BCF = 0.50

      Correction(s):   Value
       Correction Factors Not Used for Log Kow < 1

   Estimated Log BCF = 0.500 (BCF = 3.162)

Volatilization From Water

Chemical Name: 4-Pyridinamine

Molecular Weight   : 94.12 g/mole
Water Solubility   : -----
Vapor Pressure   : -----
Henry's Law Constant: 2.45E-009 atm-m3/mole (estimated by Group SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	2.318E+005	2.529E+006
HALF-LIFE (days) :	9660	1.054E+005
HALF-LIFE (years) :	26.45	288.5

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
==========
   (using 10000 hr Bio P,A,S)
PROPERTIES OF: 4-Pyridinamine

Molecular weight (g/mol)	94.12
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	2.45E-009
Air-water partition coefficient	1.00198E-007
Octanol-water partition coefficient (Kow)	1.8197
Log Kow	0.26
Biomass to water partition coefficient	1.16394
Temperature [deg C]	25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.03	23.22	10000.00
-Aeration tank	0.03	23.22	10000.00
-Settling tank	0.03	23.22	10000.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	1.1E-001	100.00
Primary sludge	2.54E-002	2.7E-004	0.25
Waste sludge	1.51E-001	1.6E-003	1.51
Primary volatilization	1.34E-006	1.4E-008	0.00
Settling volatilization	3.64E-006	3.9E-008	0.00
Aeration off gas	8.97E-006	9.5E-008	0.00
Primary biodegradation	1.76E-003	1.9E-005	0.02
Settling biodegradation	5.27E-004	5.6E-006	0.01
Aeration biodegradation	6.94E-003	7.4E-005	0.07
Final water effluent	9.81E+000	1.0E-001	98.15
Total removal	1.85E-001	2.0E-003	1.85
Total biodegradation	9.22E-003	9.8E-005	0.09

Level III Fugacity Model (Full-Output):

Chem Name : 4-Pyridinamine
Molecular Wt: 94.12
Henry's LC : 2.45e-009 atm-m3/mole (Henrywin program)
Vapor Press : 0.000347 mm Hg (Mpbpwin program)
Liquid VP : 0.000361 mm Hg (super-cooled)
Melting Pt : 26.8 deg C (Mpbpwin program)
Log Kow : 0.26 (Kowwin program)
Soil Koc : 0.746 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0328	12.6	1000
Water	45.5	900	1000
Soil	54.4	1.8e+003	1000
Sediment	0.0889	8.1e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	2.46e-012	52.4	9.5	1.75	0.317
Water	1.71e-013	1.01e+003	1.32e+003	33.8	43.9
Soil	7.16e-012	606	0	20.2	0
Sediment	1.65e-013	0.22	0.0515	0.00734	0.00172

Persistence Time: 965 hr
Reaction Time: 1.73e+003 hr
Advection Time: 2.18e+003 hr
Percent Reacted: 55.8
Percent Advected: 44.2

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air: 12.57
   Water: 900
   Soil: 1800
   Sediment: 8100
     Biowin estimate: 2.642 (weeks-months)

Advection Times (hr):
   Air: 100
   Water: 1000
   Sediment: 5e+004
